

Simulating Solute Transport in Porous Media Using Model Reduction Techniques

Bruce A. Robinson^a, Zhimimng Lu^b, Donatella Pasqualini^b

^a*Earth and Environmental Sciences Division, MS D446, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

^b*Computational Earth Sciences Group (EES-16), MS T003, Los Alamos National Laboratory, Los Alamos, NM 87545*

Abstract

In this study, we introduce a numerical method to reduce the original transport equations into a reduced form that can replicate the behavior of the original model. The basic idea is to collect an ensemble of data of state variables (say, solute concentration), called snapshots, by running the original model, and then use the proper orthogonal decomposition (POD) techniques (or the Karhunen-Loeve decomposition) to create a set of basis functions that span the snapshot collection. The snapshots can be reconstructed using these basis functions. The solute concentration at any time and location in the domain is expressed as a linear combination of these basis functions, and a Galerkin procedure is applied to the original model to obtain a set of ordinary differential equations for the coefficients in the linear representation. The accuracy and computational efficiency of the reduced model have been demonstrated using several one-dimensional and two-dimensional examples with variable permeability field K_s and sorption coefficient K_d .

Key words: Model reduction, solute transport, proper orthogonal decomposition

1. Introduction

Accurate predictions of radionuclide transport in general come from process models, which are defined as detailed flow and contaminant transport model that best replicate the available data for a site. They usually are the most complex and sophisticated models of flow and transport at a particular

6 site. A significant technical issue arises when one tries to use those model
7 results in probabilistic systems modeling: it is impractical to directly solve
8 the computationally intensive model for each Monte Carlo realization that
9 would be necessary to properly span the range of uncertainty for every model
10 parameter.

11 On contrast to process models, systems models have been proposed to
12 represent complex process models with simplified models that are suitable
13 for Monte Carlo analysis. Systems models incorporate streamlined versions
14 of one or more process models, along with uncertain estimates of the contam-
15 inant source term. Systems models integrate knowledge of all of the processes
16 relevant to assessing risk, and therefore are critical to support remedies or de-
17 cisions to monitor groundwater. Process models synthesize knowledge of one
18 component of the transport path; the systems models integrate knowledge of
19 all aspects of contaminant transport.

20 The groundwater pathway in the systems model should be an abstraction
21 model that we believe captures the essential features of the groundwater pro-
22 cess model, although there is a risk that the simplification process will filter
23 out something important. When the groundwater pathway is simulated in
24 a process model, it is generally not practical to embed the entire model in
25 the systems model - computational limitations intercede. Consequently, we
26 often settle for one or a few simplified models. These simplified models are
27 called abstraction models. Within these simplified or other types of transport
28 modules, parameters that can be varied in a probabilistic analysis include the
29 groundwater velocity, dispersion coefficient, and sorption parameters. In the
30 best case, the process model is used to justify these parameter distributions,
31 but often this is not done in great detail due to the complexity of the process
32 models and the lack of a convenient tool to formally abstract the process
33 model results. The result may be a systems model that does not fully con-
34 sider, or indeed even contradicts, one or more of the process models. The
35 credibility of the systems model is placed in jeopardy when this happens.

36 If an efficient and accurate model abstraction procedure can be imple-
37 mented for groundwater contaminant transport, we largely avoid the issue of
38 justifying the validity of our abstraction model: the original process model
39 is effectively incorporated in the systems model. Alternatively, if a model-
40 ing analysis stops short of systems analysis, the reduced model can still be
41 used to explore uncertainties much more efficiently, thereby allowing better
42 sensitivity analyses to be conducted.

43 To date, methods for proceeding from complex process models to simpli-

44 fied systems models have not been formally determined or defined. In this
 45 study a method is being developed to obtain efficient and accurate reduced
 46 models, alternatively referred to as abstraction models. The technique, called
 47 the proper orthogonal decomposition (POD), also known as principal compo-
 48 nent analysis or Karhunen-Loeve expansion, uses the results from a process
 49 model as “data” that provides the basis for a reduced model. The procedure,
 50 in general terms, calls for the running of the process model, in this case a
 51 contaminant transport simulation, forward in time, recording “snapshots”
 52 of contaminant concentration. The mathematical technique transforms the
 53 results into a set of basis functions that span the behavior of the trans-
 54 port problem throughout the model domain. The reduced model is then
 55 constructed by assuming that the solution of the transport problem can be
 56 formulated as a linear combination of the basis functions. A Galerkin proce-
 57 dure using the basis functions results in a small set of ordinary differential
 58 equations that are solved in time.

59 There are a variety of applications in various fields of science for which
 60 this technique has been applied. For example, researchers in the field of fluid
 61 dynamics have used POD methods to discern so-called coherent structures
 62 within a turbulent flow field [*Berkooz et al.*, 1993], and to characterize the
 63 spatio-temporal patterns in two-phase, fluidized bed reactors [*Cizmas et al.*,
 64 2003]. Due to the need for compact models suitable for integration into
 65 process control systems, the techniques have been applied to the modeling
 66 of non-linear heat transfer [*Park and Cho*, 1996], natural convection [*Ly and*
 67 *Tran*, 1999], and transport of chemicals in chemical vapor deposition (CVD)
 68 reactors [*Newman*, 1996b; *Ly and Tran*, 1998]. In the field of groundwater
 69 hydrology and reservoir engineering, techniques to develop reduced models
 70 have been explored [*Markovinovic et al.*, 2002; *Hejin et al.*, 2003; *Vermeulen*
 71 *et al.*, 2004], although these applications focus on fluid flow rather than
 72 contaminant transport.

73 An excellent summary of the underpinning theoretical development of
 74 POD is presented by *Newman* [1996a], and several of the aforementioned
 75 references contain detailed descriptions of the implementation of the POD
 76 technique. Of greatest relevance in the present study are the CVD model
 77 studies [*Newman*, 1996b; *Ly and Tran*, 1998]. In these models, fluid flow
 78 (a carrier gas) is assumed to be at steady state, and a reacting chemical
 79 species is transported in the fluid. Except that the flow is compressible in
 80 the CVD case, this is analogous to the problem of chemical transport in
 81 groundwater. Thus, although the POD technique has not been developed

82 for contaminant transport in groundwater, the scope of work required to
 83 develop this capability is reasonably constrained due to this previous work.

84 2. Transport Equations

85 The governing equation for transport of a single solute in porous media
 86 can be written as [Zyvoloski *et al.*, 1997]

$$87 \quad \frac{\partial(\phi S_l \rho_l C)}{\partial t} = \nabla \cdot [\phi S_l \mathbf{D} \nabla(\rho_l C)] - \nabla \cdot (\mathbf{u}_l \rho_l C) - \rho_r \frac{dC_r}{dt} + q, \quad (1)$$

88 subject to an initial condition $C(\mathbf{x}, 0) = C_0(\mathbf{x})$ and appropriate boundary
 89 conditions. Here ϕ is the porosity, S_l is the liquid saturation, ρ_l is the liquid
 90 density, C is the solute concentration, \mathbf{D} is the dispersion tensor, \mathbf{u}_l is the
 91 Darcy velocity, C_r represents the adsorption of the solute onto the porous
 92 media, $\rho_r \partial C_r / \partial t$ is an equilibrium sorption term, and q is sources or sinks. All
 93 parameters in (1) can be space-dependent, but for simplicity the coordinate
 94 $\mathbf{x} = (x_1, x_2, x_3)^T$ has been suppressed. The general equilibrium model for
 95 adsorption of species onto the porous media is given by [Polzer *et al.*, 1992]:

$$96 \quad C_r = \frac{\alpha_1 C_l^\beta}{1 + \alpha_2 C_l^\beta}, \quad (2)$$

97 where α_1 , α_2 , and β are parameters defining different sorption-isotherm mod-
 98 els. In this study, the linear isotherm model ($\alpha_1 = K_d$, $\alpha_2 = 0$, and $\beta = 1$)
 99 is used: $C_r = K_d C_l$, where K_d is the partition or distribution coefficient.

100 If we assume that flow is in saturated porous media at the steady state
 101 condition, it follows that that ρ_l , \mathbf{D} , and \mathbf{u}_l are independent of time and
 102 $S_l \equiv 1$. We may also assume that ρ_l is a constant. In this case, (1) can be
 103 simplified as

$$104 \quad \frac{\partial C}{\partial t} = \frac{\rho_l}{\phi \rho_l + \rho_r K_d} \{ \nabla \cdot [\phi \mathbf{D} \nabla(C)] - \nabla \cdot (\mathbf{u}_l C) + q \}. \quad (3)$$

105 This is the full model we deal with in this study. Given appropriate initial and
 106 boundary conditions, as well as other parameter fields such as permeability,
 107 one can first solve for the velocity field and then the concentration field from
 108 (3).

109 3. Proper Orthogonal Decomposition (POD)

110 Let $C_i(\mathbf{x}) = C(\mathbf{x}, t_i)$, $i = \overline{1, N_s}$, denote a set of N_s observations (or
 111 snapshots) of a state variable (in this case, solute concentration) observed or
 112 simulated from the full model run at time t_i , $i = \overline{1, N_s}$. The basic idea of
 113 the POD method is to find function $\psi(\mathbf{x})$, called basis functions, that have a
 114 structure typical of the members of the ensemble $C_i(\mathbf{x})$. The basis functions
 115 are chosen to give the best representation of the ensemble of snapshots, which
 116 maximizes

$$117 \quad \frac{1}{N_s} \sum_{i=1}^{N_s} |(C_i(\mathbf{x}), \psi(\mathbf{x}))|^2 / (\psi(\mathbf{x}), \psi(\mathbf{x})), \quad (4)$$

118 where (C_i, ψ) is the inner product of the basis function ψ and the concentra-
 119 tion field C_i . It can be shown that the basis functions can be expressed as a
 120 linear combination of snapshots [*Newmana*, 1996]:

$$121 \quad \psi_n(\mathbf{x}) = \sum_{k=1}^{N_s} f_{kn} C_k(\mathbf{x}), \quad k = \overline{1, N_s}, \quad (5)$$

122 where f_{kn} is the k^{th} component of the n^{th} eigenvector of the kernel \mathbf{K} that
 123 is computed from

$$124 \quad K_{ij} = \frac{1}{N_s} \int_{\Omega} C_i(\mathbf{x}) C_j(\mathbf{x}) d\mathbf{x}. \quad (6)$$

125 By equation (5), each snapshot can be reconstructed exactly using these basis
 126 functions as

$$127 \quad C_k(\mathbf{x}) = \sum_{i=1}^{N_s} f_{ki} \psi_i(\mathbf{x}). \quad (7)$$

128 To summarize, for a given ensemble of N_s snapshots, one first computes the
 129 kernel \mathbf{K} from (6) and solves the eigenproblem $\mathbf{K}\mathbf{f} = \lambda\mathbf{f}$, which gives N_s
 130 eigenvalues λ_n , $i = \overline{1, N_s}$, sorted from largest to smallest, and their cor-
 131 responding eigenfunctions $f_n(\mathbf{x})$, $i = \overline{1, N_s}$. The basis functions are then
 132 computed from (5) and any snapshot can be reconstructed using (7). Since
 133 the matrix \mathbf{K} is real, symmetric and positive semi-definite, all eigenvalues
 134 are non-negative. The importance of the n^{th} eigenfunction depends on its
 135 relative “energy”, characterized by the ratio of the n^{th} eigenvalue to the sum
 136 of all eigenvalues (total energy): $\lambda_n / \sum_{i=1}^{N_s} \lambda_i$. In many cases, the first few
 137 eigenvalues carry most of the total energy and thus concentration $C(\mathbf{x})$ in
 138 (7) can be approximated by truncating the first M terms ($M \ll N_s$).

139 To find the spatial distribution of concentration at a time that is not in
 140 the ensemble of snapshots, one has to solve for the coefficients in (7). In the
 141 following section, a reduced model is introduced, in which ordinary differ-
 142 ential equations for these coefficients are derived from the original (partial
 143 differential) transport equations.

144 4. Reduced Model

145 Suppose that the full model (3) is solved to obtain a set of snapshots of
 146 the concentration distribution $C(\mathbf{x}, t_i)$, $i = \overline{1, N_s}$. Based on the algorithm
 147 described in the previous section, one can find a set of basis functions $\psi_i(\mathbf{x})$,
 148 $i = \overline{1, N_s}$. Then a Galerkin's method can be employed by seeking an approx-
 149 imation of concentration $C(\mathbf{x}, t)$ as

$$150 \quad \hat{C}(\mathbf{x}, t) = \sum_{m=1}^M a_m(t) \psi_m(\mathbf{x}), \quad (8)$$

151 where $M < N_s$, and $a_m(t)$ are time-varying coefficients that are indepen-
 152 dent of spatial locations. The physical mean of (8) is that the concentra-
 153 tion field is approximated by a linear combination of some pre-determined,
 154 space-dependent “structures” weighted by time-dependent coefficients. Since
 155 $\hat{C}(\mathbf{x}, t)$ in (8) is an approximation of the true concentration, replacing $C(\mathbf{x}, t)$
 156 in the full model, i.e., transport equation (3), by $\hat{C}(\mathbf{x}, t)$ will in general pro-
 157 duce a model error. In the Galerkin's method, this error is forced to be
 158 orthogonal to all these basis functions, i.e.,

$$159 \quad \int_{\Omega} \left[\frac{\partial \hat{C}}{\partial t} - \frac{\rho_l}{\phi \rho_l + \rho_r K_d} \left\{ \nabla \cdot [\phi \mathbf{D} \nabla \hat{C}] - \nabla \cdot (\mathbf{u}_l \hat{C}) + q \right\} \right] \psi_i(\mathbf{x}) d\mathbf{x} = 0, \quad (9)$$

160 for $i = \overline{1, M}$. Here the orthogonality of two functions $f(\mathbf{x})$ and $g(\mathbf{x})$ is
 161 defined as $\int_{\Omega} f(\mathbf{x}) g(\mathbf{x}) d\mathbf{x} = 0$. Substituting (8) into (9) and recalling the
 162 orthogonality of basis functions yield

$$\begin{aligned} \frac{da_i(t)}{dt} &= \sum_{j=1}^M a_j(t) \frac{\rho_l}{\phi \rho_l + \rho_r K_d} \int_{\Omega} \{ \nabla \cdot [\phi \mathbf{D} \nabla (\psi_j(\mathbf{x}))] - \nabla \cdot [\mathbf{u}_l \psi_j(\mathbf{x})] \} \psi_i(\mathbf{x}) d\mathbf{x} \\ &+ \int_{\Omega} \frac{q(\mathbf{x}, t) \psi_i(\mathbf{x})}{\phi \rho_l + \rho_r K_d} d\mathbf{x}, \end{aligned} \quad (10)$$

163 which can be written in a matrix form as

$$164 \quad \frac{dA(t)}{dt} = B A(t) + Q(t), \quad (11)$$

165 where $A = (a_1, a_2, \dots, a_M)^T$, matrix $B = (b_{ij})_{M \times M}$ and vector $Q = (q_i)_{M \times 1}$
 166 are defined as

$$167 \quad b_{ij} = \frac{\rho_l}{\phi \rho_l + \rho_r K_d} \int_{\Omega} \{ \nabla \cdot [\phi \mathbf{D} \nabla (\psi_j(\mathbf{x}))] - \nabla \cdot [\mathbf{u}_l \psi_j(\mathbf{x})] \} \psi_i(\mathbf{x}) d\mathbf{x}, \quad i, j = \overline{1, M}, \quad (12)$$

168 and

$$169 \quad q_i(t) = \frac{1}{\phi \rho_l + \rho_r K_d} \int_{\Omega} q(\mathbf{x}, t) \psi_i(\mathbf{x}) d\mathbf{x}, \quad i = \overline{1, M}. \quad (13)$$

170 The initial condition for (11) is derived from the original initial condition
 171 $C(\mathbf{x}, t) = C_0(\mathbf{x})$,

$$172 \quad a_i(0) = \int_{\Omega} C(\mathbf{x}, 0) \psi_i(\mathbf{x}) d\mathbf{x}, \quad i = \overline{1, M}. \quad (14)$$

173 Thus the partial differential equation (PDE) has been reduced to a system
 174 of M ordinary differential equations (ODE). Provided that M is fairly small,
 175 the reduction in computational time should be significant compared to the
 176 numerical solution of the PDE in the original model.

177 5. Illustrative Examples

178 In this section, several examples are presented to illustrate how the model
 179 reduction techniques can significantly reduce computational efforts in solute
 180 transport in porous media, while retaining accuracy. This is accomplished by
 181 comparing results from the reduced models against those from the full model
 182 runs. Note that, in solving the full model numerically, it is quite often that
 183 numerical errors may be introduced. To avoid this, in the first two examples,
 184 simple one-dimensional transport problems were chosen because analytical
 185 solutions for these simple cases are available, which made it easy to assess
 186 the accuracy of the reduced model.

187 *5.1. One-dimensional solute transport with linear sorption*

188 In the first example, we consider a one-dimensional transport problem in a
 189 saturated column of $1m$ in length, uniformly discretized into 200 elements.
 190 The hydraulic conductivity is a constant $K_s = 1.0 \text{ m/day}$ for the entire
 191 column, and the flow is driven by a hydraulic gradient of $dh/dx = 0.001$,
 192 which produces a uniform flow with Darcy velocity of $1.1813 \times 10^{-8} \text{ m/s}$.
 193 Other transport parameters are given as: the dispersivity coefficient $\alpha_L =$
 194 0.03333 m , partition coefficient $K_d = 0.1$, water density $\rho_l = 1000.0 \text{ kg/m}^3$,
 195 rock density $\rho_r = 2500 \text{ kg/m}^3$, and porosity $\phi = 0.25$. Under the given
 196 initial condition $C(x, 0) = 0$, a fixed concentration $C(x, t) = 1.0$ at the inlet
 197 ($x = 0$), and a zero concentration gradient $\partial C(x, t)/\partial x = 0$ at $x = \infty$, this
 198 problem can be solved analytically [Batu, 2006]:

$$199 \quad C(x, t) = \frac{1}{2} \operatorname{erfc} \left[\frac{x - vt/R}{\sqrt{4\alpha_L vt/R}} \right] + \frac{1}{2} \exp \left(\frac{x}{\alpha_L} \right) \operatorname{erfc} \left[\frac{x + vt/R}{\sqrt{4\alpha_L vt/R}} \right], \quad (15)$$

200 where $R = 1 + \rho_r K_d / (\phi \rho_l)$ is the retardation factor, and erfc is the comple-
 201 mentary error function. Twenty-five concentration snapshots are computed
 202 using (15) at time $t = n\Delta t$, where $\Delta t = 20 \text{ days}$ and $n = \overline{1, 25}$. Some
 203 selected snapshots are illustrated in Figure 5.

204 Using these 25 snapshots, the kernel \mathbf{K} is computed from (6), and the
 205 eigenvalues and eigenfunctions associated with this kernel are solved from
 206 $\mathbf{K}\mathbf{f} = \lambda\mathbf{f}$. These eigenvalues and eigenfunctions depend significantly on the
 207 choice of snapshots. It is critical that each snapshot be significantly different
 208 from all others. The eigenvalues for this set of snapshots are depicted in
 209 Figure 5.1. The figure indicates that the first eigenvalue carries about 91%
 210 of the total energy and the first 6 eigenvalues carry more than 99.99% of
 211 the total energy. The ratio of the accumulative energy to the total energy
 212 is a measure that can be used to determine the number of modes needed to
 213 achieve a given accuracy.

214 The first few basis functions are illustrated in Figure 5.1. It is seen
 215 from the figure that the magnitude of the first basis function is much larger
 216 than that of other basis functions. In addition, the magnitude decreases
 217 as the mode number increases, which makes it possible to approximate the
 218 concentration field using only a few terms rather than $N_s (= 25)$ terms.

219 Based on these basis functions, all snapshots can be reconstructed using
 220 (7). Comparisons of the true snapshots and reconstructed snapshots indicate
 221 that at most 6 basis functions are enough to reconstruct these snapshots
 222 with sufficient accuracy. Of course, in general, the number of basis functions
 223 required to obtain an accurate solution will depend on the parameters (K_s ,
 224 α_L , and L) in the solute transport problem.

225 The spatial distribution of solute concentration at any give time can be
 226 derived from solving the reduced model. The ordinary differential equation
 227 (11) with initial condition (14) was solved using the fourth-order Runge-
 228 Kutta method with a time step of $\Delta\tau = 1000$ s. In particular, the ensemble
 229 of those snapshots can be solved from the reduced model (rather than recon-
 230 structed from (7)). Four selected concentration distributions computed from
 231 the reduced model, as functions of the number of basis functions included,
 232 are illustrated in Figure 5.1. Also plotted in the figure is the true (exact)
 233 solution from (15). The figure clearly shows that the accuracy of the esti-
 234 mated concentration distribution depends on the number of basis functions
 235 included. For this example, including 10 basis functions is enough to produce
 236 very accurate results as compared to the exact solutions.

237 It is interesting to investigate how well the reduced model can predict
 238 the concentration distribution at an elapsed time that is different from those
 239 times at which the ensemble of snapshots are taken. Figure 5.1 compares
 240 the concentration profiles at time $t = 75$ and 525 days computed from the
 241 analytical solution and those solved from the reduced model with 15 basis
 242 functions. Note that $t = 525$ days is larger than the maximum time of all
 243 snapshots used in constructing the reduced model. The comparison in the
 244 figure demonstrates that the reduced model can reproduce the true solution
 245 accurately.

246 5.2. One-dimensional transport with pulse input

247 In the second example, all transport parameters are the same as in the pre-
 248 vious example except that (1) the partition coefficient K_d is zero in this case,
 249 and (2) instead of a fixed constant concentration at the inlet ($x = 0$), a unit
 250 pulse input is imposed at the inlet for a duration of 5 days. For this simple

251 case, analytical solution is also available [Batu, 2006]

$$\begin{aligned}
252 \quad C(x, t) &= \frac{1}{2} \operatorname{erfc} \left[\frac{x - vt}{\sqrt{4\alpha_L vt}} \right] + \frac{1}{2} \exp \left(\frac{x}{\alpha_L} \right) \operatorname{erfc} \left[\frac{x + vt}{\sqrt{4\alpha_L vt}} \right] \\
253 \quad &- \frac{1}{2} \operatorname{erfc} \left[\frac{x - v(t - t_0)}{\sqrt{4\alpha_L v(t - t_0)}} \right] - \frac{1}{2} \exp \left(\frac{x}{\alpha_L} \right) \operatorname{erfc} \left[\frac{x + v(t - t_0)}{\sqrt{4\alpha_L v(t - t_0)}} \right] \quad (6)
\end{aligned}$$

254 where t_0 is the duration of the pulse input, which starts at zero. Using
255 this equation, 25 snapshots were calculated from $t = 10$ to 250 days at an
256 increment of 10 days. Several selected snapshots are illustrated in Figure 5.2.

257 Following the POD method, the kernel K was computed from these 25
258 snapshots using (6); eigenvalues and eigenfunctions were solved from the
259 eigenproblem $\mathbf{Kf} = \lambda \mathbf{f}$; and then basis functions were computed using (5).
260 The set of eigenvalues as a function of the mode is depicted in Figure 5.2. Un-
261 like the previous case where the first eigenvalue carries about 90% of energy,
262 in this case the first one has only 40% of energy and the first 8 eigenvalues
263 carry about 99.99% energy, which means that more basis functions may be
264 required to approximate the solution. This can also be seen from Figure 5.2,
265 where the relative magnitudes of the first few eigenfunctions are more or less
266 the same, while in the previous example the magnitude of the first eigen-
267 function is much larger than that of other eigenfunctions. A larger number
268 of required basis functions may be attributed to the fact that the patterns of
269 different snapshots are quite different in this example while in the previous
270 example all snapshots have a very similar pattern.

271 Figure 5.2 compares four snapshots computed from the analytical solution
272 and those solved from the reduced model with different numbers of basis
273 functions included in the reduced model. It is seen from the figure that the
274 reduced model with 10 basis functions is accurate enough. Figure 5.2 shows
275 the comparison of concentration profiles at time $t = 75$ and 275 days derived
276 from the analytical solution and those from solving the reduced model with
277 10 basis functions. Again, the solutions from the reduced model are nearly
278 identical to the true solutions.

279 5.3. Two-dimensional solute transport with heterogeneous permeability and
280 sorption coefficients

281 In the third example, solute transport is modeled in a two-dimensional rect-
282 angular domain of size $1\text{ m} \times 0.5\text{ m}$, uniformly discretized into 100×50 square
283 elements. No-flow conditions are prescribed at two lateral boundaries. The
284 hydraulic head is fixed at the left and right boundaries as 10.001 m and 10.0 m ,
285 respectively, with a hydraulic gradient $J = 0.001$. The porous medium is
286 heterogeneous in both the hydraulic conductivity K_s and the sorption coeffi-
287 cient K_d . It is assumed that the log hydraulic conductivity $Y = \log(K_s)$ has
288 a normal distribution and is second-order stationary following an isotropic,
289 exponential covariance function with a correlation length of 0.3 m . The
290 statistics of the log hydraulic conductivity are given as $\langle Y \rangle = 0$, (i.e., the
291 geometric mean of the saturated hydraulic conductivity $K_G = 1.0\text{ m/day}$)
292 and $\sigma_Y^2 = 0.693$ (coefficient of variation $CV_{K_s} = 100\%$). Figure 5.2a shows
293 the log hydraulic conductivity field generated using the *sgsim* code in GSLIB
294 [Deutch and Journel, 1998]. In this case, the velocity field is no longer uni-
295 form in the flow domain and has to be solved numerically. The steady-state,
296 saturated flow problem was solved using the Finite-Element Heat- and Mass-
297 Transfer code (FEHM) developed by Zyvoloski *et al.* [1997]. This velocity
298 field was used as input to the solute transport model.

299 For the transport problem, it is assumed that the initial concentration
300 is zero in the domain and concentration of $C(\mathbf{x}, t) = 1.0$ is fixed at the
301 middle of the upstream boundary, $(0.0\text{ m}, 0.25\text{ m})$. It is also assumed the
302 log partition coefficient is uncorrelated with the log hydraulic conductivity
303 and that $\ln(K_d)$ is also second-order stationary field following an isotropic,
304 exponential covariance function with a correlation length of 0.3 m . The
305 statistics of $\log(K_d)$ are given as $\langle \ln(K_d) \rangle = -1.6094$, (i.e., the geometric
306 mean $K_d^G = 0.2$) and $\sigma_{\ln K_d}^2 = 9.95 \times 10^{-3}$ (coefficient of variation $CV_{K_d} =$
307 10%). The spatial distribution of K_d generated using the *sgsim* code of
308 GSLIB is illustrated in Figure 5.2b. Other transport parameters include
309 the longitudinal dispersivity coefficient $\alpha_L = 0.02\text{ m}$, and the transverse
310 dispersivity coefficient $\alpha_T = 10^{-4}\text{ m}$.

311 The full transport model was run for 200 days using the FEHM code
312 and the concentration distribution was recorded at $t = 10n$ days, where

313 $n = \overline{1, 20}$, and these 20 concentration fields were taken as snapshots for the
 314 model reduction method. Basis functions were then computed from these
 315 snapshots using the POD method, and equation (11) with initial condition
 316 (14) were solved numerically.

317 Figure 5.3 compares the spatial distribution of concentration as contour
 318 maps at two elapsed times, $t = 100$ days and $t = 200$ days, derived from
 319 both the full model run and the reduced model with 5 basis functions. The
 320 comparison clearly shows that the results from the reduced model can re-
 321 produce the full model results very well, even for a contour level as low as
 322 $C = 0.01$.

323 To compare the computational efficiency of these two methods, the CPU
 324 time required for the full model run was recorded, in which the maximum
 325 time step was set to 2 days while the actual size of the time step was auto-
 326 matically adjusted during the solution process by the program itself. For the
 327 transport problem as described above, the FEHM code takes 23.3 hours. The
 328 computation time needed for the reduced model depends on the time step
 329 used in the fourth-order Runge-Kutta method, which is fixed at $\Delta\tau = 1000$
 330 seconds in this case. The CPU time for the reduced model run is only 78
 331 seconds. Of course, this run time will increase if a small time step was used
 332 or a great number of snapshots and functions is required. However, the
 333 comparison of model results from the full model and the reduced model in-
 334 dicates that the time step of $\Delta\tau = 1000$ seconds used in the reduced model
 335 is small enough for this problem, and the overall comparison indicates that
 336 the number of snapshots and basis functions were sufficient.

337 For the purpose of comparison, an additional example was simulated, by
 338 setting $K_d = 0$ in the previous example. In this case, the plume moves
 339 faster than in the third example. As shown in Figure 5.3, comparison of the
 340 concentration fields derived from the full model and the reduced model at
 341 times $t = 50$ days and $t = 100$ days also demonstrates that the reduced
 342 model can reproduce the full model results with a sufficient accuracy.

343 6. Conclusions

344 In this study, we have demonstrated that the advection-dispersion equa-
 345 tion can be cast in reduced model form, and a reduced numerical model can
 346 be developed that replicates the behavior of the original model. We have de-
 347 rived, from the original model equations, a method for reducing the transport

348 model, a partial differential equation with unknowns at each numerical grid
 349 point, to a small number of ordinary differential equations solved in time.
 350 The method consists of running the original model to obtain the snapshots
 351 of concentration in the model domain, computing the basis functions for the
 352 model using the POD technique, and using these basis functions in a Galerkin
 353 procedure to obtain the ordinary differential equations of the reduced model.
 354 The accuracy and computational efficiency of the reduced model have
 355 been investigated using several one-dimensional and two-dimensional exam-
 356 ples with variable permeability field K_s and sorption coefficient K_d . These
 357 examples demonstrate that the reduced model can reproduce the full model
 358 results very accurately while the computational time (in terms of the CPU
 359 time) required for the reduced model is much less than that required for the
 360 full model.

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Figure Captions

Figure 1. Selected snapshots computed from Equ. (15) for the one-dimensional solute transport with linear sorption.

Figure 2. The eigenvalues and their accumulative value as functions of modes for the one-dimensional solute transport with linear sorption.

Figure 3. Selected basis functions for the solute transport with linear sorption.

Figure 4. Accuracy of computed snapshots using the model reduction method with different numbers of basis functions for the one-dimensional solute transport with linear sorption.

Figure 5. Comparison of exact solution and reduced model solution at time $t = 75$ days and 525 days for the one-dimensional solute transport with linear sorption.

Figure 6. Selected snapshots computed from (16) the one-dimensional solute transport with pulse input.

Figure 7. The eigenvalues and their accumulative value as functions of modes for the one-dimensional solute transport with pulse input.

Figure 8. Selected basis functions for the one-dimensional solute transport with pulse input.

Figure 9. Accuracy of computed snapshots with different numbers of basis functions using the model reduction method for the one-dimensional solute transport with pulse input.

Figure 10. Comparison of exact solution and reduced model solution at time $t = 75$ days and 275 days for the one-dimensional solute transport with pulse input.

Figure 11. Gaussian random fields for (a) $\log K_s$, and (b) K_d .

Figure 12. Comparison of true concentration fields and modeled fields using the reduced model at two elapsed times for the case with heterogeneities in both the permeability and the distribution coefficient.

Figure 13. Comparison of true concentration fields and modeled fields using the reduced model for two elapsed times for the case with heterogeneous permeability field but without sorption ($K_d = 0$).